

## PROCESS FOR PREPARING HIGH PURITY TNT

Background of the Invention1. Field of the Invention

The present invention relates to organic chemistry and more particularly to the processing of aromatic hydrocarbons. Still more particularly, the present invention relates to processes for preparing trinitrotoluene (TNT).

2. Brief Description of Prior Developments

In the prior art process of preparing TNT, one mole of 2,4-dinitrotoluene is added to a mixture of 3 moles of concentrated nitric acid and 5 moles of concentrated sulfuric acid. The mixture is heated to 130° C for 2 hours. The dark red brown viscous solution is poured into a large volume of water and the crude TNT product is isolated by filtration, then purified by washing with sodium sulfite solution which affords a "red water" waste containing TNT isomers and impurities. The TNT is then washed with hot water. The yield of TNT is approximately 84%

A disadvantage of this prior art process is due to the fact that a large volume of concentrated sulfuric acid is used. The acid mixture is highly corrosive. The initial crude TNT is impure and must be purified by sulfite washing which produces a environmentally hazardous waste. The resulting large volume of spent sulfuric acid must be ~~recovery~~ recovered and purified for reuse.

### Summary of Invention

An object of the present invention is to overcome the limitations of the prior art methods requiring large quantities of strong oxidizing acids such as sulfuric acid while maintaining an economically useful process.

Another object of the present invention is to avoid producing the environmentally hazardous "red water" waste stream which is created with other methods.

In the process of the present invention, TNT is prepared in high purity by either a two step process beginning with toluene or alternatively a one step process starting with dinitrotoluene.

Toluene reacts with 90 - 99% nitric acid and preferably 98-99% nitric acid at  $<60^{\circ}\text{C}$  and preferably  $<30^{\circ}\text{C}$  to afford a high yield of high purity dinitrotoluene (DNT) at a purity of 99% by weight. The DNT which can be readily converted to TNT by heating this material with a mixture of 98-99% nitric acid in the presence of only one equivalent of the non-oxidizing acid, trifluoromethanesulfonic acid. The process affords very high purity TNT having a purity of  $>99\%$  by weight.

Unless otherwise stated, all concentrations herein are by weight.

### Detailed Description of the Present Invention

→ In the present invention TNT is prepared from toluene or 2,[[2]] 4-dinitrotoluene by the following reactions.

